2-Chloronaphthalene 91-58-7 | DTXSID8023971

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.81	0.55	0.81	0.54	0.71	0.61	

Model Results

Predicted value: 1620 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.20e-01

Confidence level: 7.12e-01

Nearest Neighbors from the Training Set

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2-Methylnaphthalene Measured: 3980 Predicted: 2000

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1-Naphthol Measured: 525 Predicted: 1720

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Biphenyl Measured: 1860 Predicted: 2430

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Chloroneb Measured: 1260 Predicted: 199

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1-Methylnaphthalene Measured: 2290 Predicted: 1860